

## **AFOSR Final Progress Report – 2005**

### **CHSSI: Scalable Software for Bridging Atomistic and Continuum Simulations**

(Grant # F49620-02-1-0190)

Principal Investigator: Gregory A. Voth  
Department of Chemistry  
University of Utah  
Salt Lake City, Utah 84112

#### **Objectives:**

The final developments of a scalable mesoscale dynamics simulation TANTALUS are summarized.

#### **Status of Effort:**

The primary effort has been on the development of massively parallel simulation codes capable of modeling both solid and viscous materials at the meso-scale. The construction of a full 3D-spatial decomposition parallel algorithm has been tested and completed. The inclusion of the ES (elastic solid) formulation within the 3D spatial decomposition has been completed. The Alpha software test was completed in June, 2003 with all CTP's met. Code development is on schedule and ongoing. The Best test was completed in July, 2004 with all requirements met. The project was accomplished successfully.

#### **Accomplishments/New Findings:**

A highly scalable spatial decomposition algorithm designed for meso-scopic simulation has been developed and tested. The core parallel architecture employs a combination cell-code/spatial decomposition algorithm that is designed to be automatically generated and optimized. Scalability tests indicate excellent scaling over system sizes on the order of a million mesoparticles over 216 processors. With the fact that one meso particle represents 100-1000 actual molecules, and that TANTALUS can model systems on the order of a microsecond on large platforms, the real time viability of attaining macro-scale spatial and temporal phenomena are now possible.

In Fig. 1, the scaling results for a large meso-scopic system up to 216 processors are excellent. A new 6 way communication scheme has recently been implemented within the spatial decomposition algorithm. With this new communication sequence, the cost of processors communication is almost nil. System sizes requiring 1000 processors and beyond are now feasible.

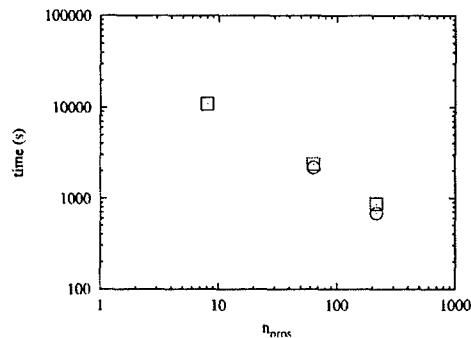
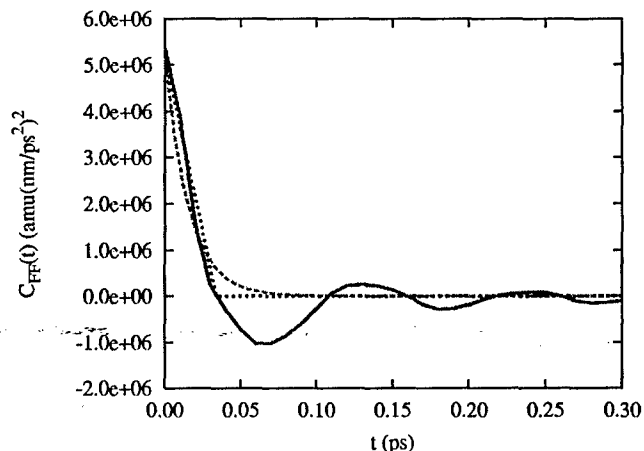


Fig. 1. Scaling results for TANTALUS. The ratio  $t(2n)/t(n)=1.7$ .

Additionally, in order to construct a robust micro-meso feedback mechanism, a reformulation of coarse-grained nanoscale fluid dynamics was required. The reformulation has been successful, and has resulted in the first computationally feasible, systematic bridged method to model complex systems as the mesoscale. Implementation of the full micro-meso interface is now underway. In Fig. 2, the complete force-force TCF for meso-water is shown using the coarse-grained TANTALUS simulation. The different curves correspond to different degrees of the coarse-grained resolution of the model.

Fig. 2 force-force mesoscale interactions.



The mesoscale dynamics methodology, denoted BLOB/BLOBs, has the capability of modeling soft matter at mesoscopic levels *without* resorting to *ad-hoc* models. Length constraints do not allow for a complete description of the BLOB/BLOBs methodology, but as a summary we have already found that the transition between atomistic-level dynamics in condensed phases (characterized typically by strong “caged” correlations in particle velocities) to continuum-level fluid dynamics (where no molecular-level structure is resolved) occurs through a well defined mesoscopic regime where the dynamics contains characteristics of both. Fig. 3 show a mesoscale BLOB particle employing the EM elastic-mesh designed to model elastic solids. The mesoparticle is over 100 nm in diameter and is immersed in over 1,000,000 meso-solvent particles. The solvent is not shown for clarity.

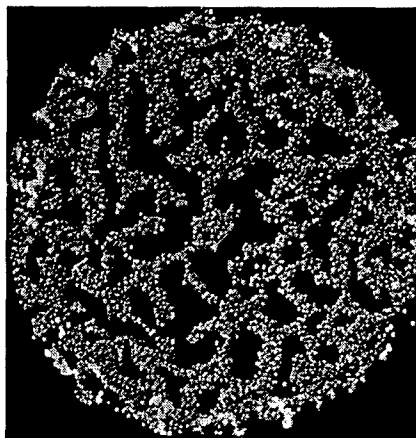


Fig. 3. A BLOB mesoparticle employing TANTALUS.

Large scale simulations employing the viscous BLOB and elastic EM model have been performed over 216 processors. The present system is designed to examine long wavelength oscillations in thin elastic membrane structures. The long time-scales attainable with the mesoscale TANTALUS simulation allow for examine of properties not accessible with MD. Simulation snapshots are shown Fig. 4.

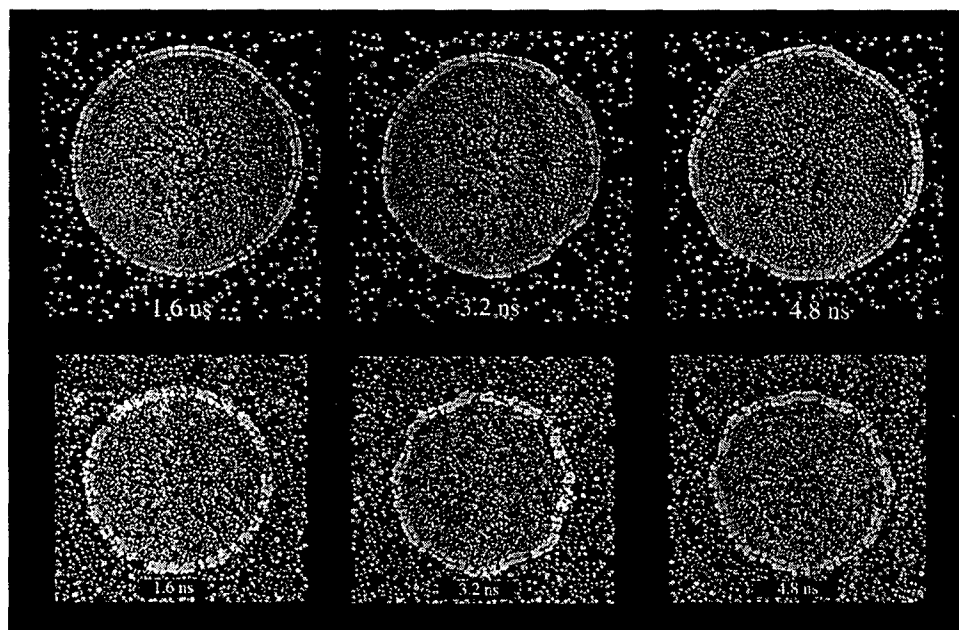


Fig. 4. Snapshots of an elastic solid membrane Immersed in a meso-solvent.

Work has already begun on applying TANTALUS to examine Ionic Liquids (ILs). The preliminary micro-scale parameterization sequence has already indicated that these systems exhibit long wavelength phenomena amenable to the TANTALUS mesoscale simulation methodology. In Fig. 5, are the dynamical resolutions of mesoscopic representations of and IL fluid.

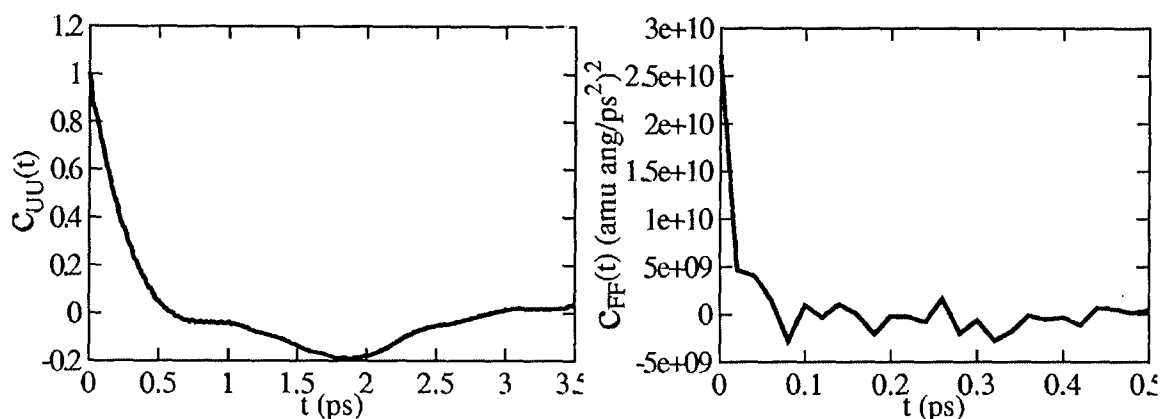


Fig. 5. Ionic Liquid mesoscale dynamics. The left panel shows The velocity-velocity correlations while the right shows the Force-force correlations.

TANTALUS has recently passed the BETA software test (July,2004). Scaling results over 216 processors on all platforms were perfect. An additional user manual has been constructed. New findings have been related to the effects of long time thermal deformations on elastic systems immersed in viscous solvents.

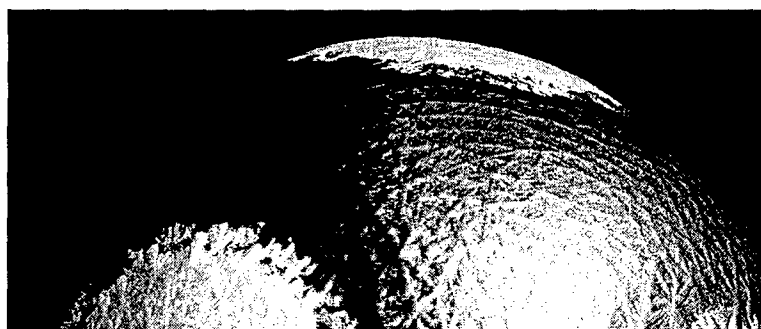


Fig. 6. Line tension perturbations in an elastic vesicle.

In Fig. 6 we show recent results where TANTALUS has been employed to examine mesoscale line-tension on elastic vesicle of diameter of 20 micrometers. Extensions to elastic filaments in viscous solvents are now underway.

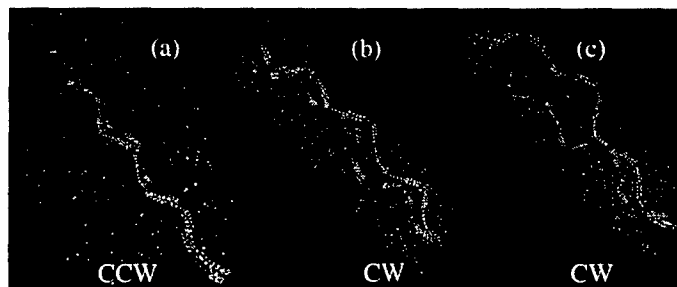


Fig. 7. Elastic filaments in a meso-solvent.

In Fig. 7, snapshot of rotating elastic filaments in a meso-solvent employing TANTALUS show interesting meso-hydrodynamic coupling to the elastic deformations.

**Personnel Supported:**

Gregory A. Voth (P.I.)  
 Gary Ayton (Research Professor)  
 Yeshitila Gebremichael (Postdoc)  
 Qiang Shi (Postdoc)  
 Jian Zhou (Postdoc)  
 Stephanie Atherton (Graduate)  
 Sun Kim (Graduate)  
 Zhen Qin (Graduate)

**Publications Related to Project:**

None. (This project is not about publications, but about software development.)

**Interactions/Transitions Related to Project:**

(a) *Participation/Presentations at Meetings, Conferences, Seminars, etc.*

None.

(b) *Consulting/Advisory Functions*

Gaussian, Inc.

(c) *Transitions*

The code will be distributed through the DoD CHSSI Program to DoD researchers when requested.

**New Discoveries, Inventions, Patents**

None

**Honors/Awards:**

None

# REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-05-

8306

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering the required data, completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188) 4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to provide information herein if it does not contain any information that is not otherwise available by other means. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

1. REPORT DATE (DD-MM-YYYY) 07/20/2005		2. REPORT TYPE AFOSR Final Progress Report		3. DATES COVERED (From - To) 05/01/2002 - 04/30/2005	
4. TITLE AND SUBTITLE CHSSI: Scalable Software for Bridging Atomistic and Continuum Simulations				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER F49620-02-1-0190	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Gregory A. Voth				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Utah Department of Chemistry 315 S. 1400 E., RM 2020 Salt Lake City, Utah 84112-0850				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 4015 NE 45 <sup>th</sup> St., STE 350 Seattle, Washington 98105-4631 University of Utah Office of Sponsored Projects 1471 E. Federal Way Salt Lake City, Utah 84102-1821				10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR OSP	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION / AVAILABILITY STATEMENT  Unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT A highly parallel simulation software capable of modeling complex systems at the mesoscale was developed and tested. The scaling of the simulation computer code, called TANTALUS, was found to be excellent, due to the novel spatial decomposition algorithm that was developed. TANTALUS was employed to examine a number of complex systems as demonstration projects.					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF: Unclassified			17. LIMITATION OF ABSTRACT 0	18. NUMBER OF PAGES 7	19a. NAME OF RESPONSIBLE PERSON Gregory A. Voth
a. REPORT 6	b. ABSTRACT 0	c. THIS PAGE 1			19b. TELEPHONE NUMBER (include area code) (801) 581-7272